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13. ABSTRACT (Maximum 200 words) This project developed computational and mathematical tools, based extensively on elements of system theory, that enable microscopic/stochastic simulators to perform system-level tasks (analysis, design, control, optimization). In current engineering modeling we are often faced with situations where the system model is given at an atomistic / stochastic / agent based level, while the modeling tasks (simulation, controller design, optimization) must be performed at a much larger, macroscopic in space and time level. The objective was to construct a bridge between existing and future microscopic simulation codes (kMC, MD, MC, BD, LB etc.) and traditional, continuum numerical analysis. To accomplish this, we traded function evaluations (in the continuum computations) for appropriately initialized "bursts" of microscopic simulations, executed over short space and time intervals, followed by post-processing based on system-identification techniques. Separation of time scales is another important ingredient of the bridge between micro-simulation and macro-modeling. We stress controller design and optimization tasks this year. We also explored how this "model on demand" approach can evolve into experimental design protocols. Several examples, from small molecule folding to complex fluid rheology and computational materials science were pursued in order to validate the approach.					
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F49620-03-1-0097

Final Report

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Abstract

This project aimed at developing computational and mathematical tools, based extensively on elements of system theory, that enable microscopic/stochastic simulators to perform system-level tasks (analysis, design, control, optimization). We stressed controller design and optimization tasks. Several examples, from small molecule folding to complex fluid rheology and computational materials science were pursued. Later important developments involved the extension of the computational technology to encompass uncertainty quantification as well as the detection of appropriate observables from data (the "variable free" component of the "equation-free" approach).

Objectives

The objective of this project was outlined in the original proposal: to enable advanced, computer-assisted analysis and design computations for complex, nonlinear, distributed (spatially varying) processes described by microscopic (atomistic, stochastic, agent-based) models. The algorithms developed as part of the project allow scientific computing tasks (like simulation, stability and bifurcation analysis, control and optimization) to be performed for problems for which the physical description is available at a "fine" microscopic or stochastic level, but the questions asked are at a macroscopic, systems level. This bridge takes the form of software "wrappers", that can be combined with state of the art microscopic simulation codes (like molecular dynamics, MD, kinetic Monte Carlo, kMC, equilibrium MC, Lattice-Boltzmann, LB, Brownian Dynamics, BD, or general agent-based, AB) simulators. It also, fortuitously, encompasses the case of large scale legacy codes, which can also be enabled by these "wrappers". System theory tools (system identification, separation of time scales) play a prominent role in this computational enabling technology.

Accomplishments

Possibly the best way to examine the accomplishments of this work is to look through the titles of publications in refereed journals (appeared, in press and submitted) that appear at the end of this final report. In the first year we performed extensive work on

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the development and implementation of computational algorithms; we have also performed extensive work on the “coarse computational study” of the dynamics of a number of physical systems (based on Brownian Dynamics, on kinetic Monte Carlo, on equilibrium Monte Carlo, on Molecular Dynamics as well as on legacy codes). We emphasized particularly the modifications that arise in the context of using coarse methods in a control context (a paper on coarse linear control of Brownian Dynamics, one on coarse linear control of lumped kinetic MC simulations, one on coarse linear control of LB distributed simulators). There is one publication on coarse, timestepper-based optimization, which is going to be submitted within a month or so; there is another paper on the “patch-dynamics” based control of distributed parameter systems that we expect to submit this calendar year. There were also several Proceedings papers which we simply did not mention (ACC, upcoming CDC etc.). In the second year we had successes in problems as diverse as evolutionary epidemiology (Cisternas et al.) and bacterial chemotaxis (Setayeshgar et al.), computational materials science (Haataja et al.) and equilibrium complex fluids (Kopelevich et al.). At the same time we proposed new links of the equation-free approach with control algorithms (Armaou et al., Siettos et al., collaboration with Christofides), the use of legacy codes (Siettos et al.); and worked on numerical analysis and new algorithms (Samaey et al., Kelley et al., Gear et al.). More recent accomplishments were made along three directions: The first was the equation-free approach to uncertainty quantification. The idea is simple: try to combine the best features of Monte Carlo sampling with the strength of the Polynomial (Wiener) chaos representation. Do short bursts of MC simulations, and use them to estimate, on the fly, the time- and parametric dependence of the appropriate observables – polynomial chaos projections of the result distributions. We already have, in addition to a first paper, another paper where the approach is used to develop algorithms for the study of homogenization problems. The second direction had to do with the coherent behavior of interacting entities (e.g. vehicles, swarms etc.). Here there are two options: are the interacting entities identical or different? If they are similar, then “traditional” equation-free methods are used – we can observe the evolution of the statistics of brief microscopic simulations, and then use our equation-free approach for accelerated modeling or control purposes. But if the interacting entities have a distribution or properties, we can again take advantage of the computational chaos observables, and evolve not the statistics of the evolving distribution, but the projection of this distribution on polynomial chaos basis functions. There have been several papers along these lines including a recent *Phys. Rev. Lett.* The third direction has to do with novel data processing methods for determining the right observables from complex, high-dimensional data. Here, in collaboration with R. Coifman at Yale, we have developed methods for linking equation-free computation with diffusion maps: a computational approach based on harmonic analysis on graphs that allows for finding the “right coarse observables” from high dimensional simulation data; and the use of these results BOTH in accelerating simulations and in bootstrapping the data collection process. Finally, the methods we developed are already naturally applied to study the control of fluctuations in nanoscopic systems – a good example is provided by the parametric study of water filling-emptying transitions in carbon nanotubes, which also appeared in *Phys. Rev. Letters*. Overall, as the techniques mature and the application

list lengthens, the methods become more visible and start to be used by other people also – there was an article about this overall work program last month in SIAM News.

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Personnel Supported

Prof. Ioannis G. Kevrekidis, the PI, was partially supported during the summers of this period. Post-doctoral research associates partially supported were Dr. Costas Siettos, Dr. Jaime Cisternas, Dr. Ligang Chen and Dr. Sung-Joon Moon. Graduate students partially supported included Mr. L. Qiao, Mr. J. Nehlsen and Ms. Joanne Chia; the latter two have graduated with PhD degrees, and the former is expected to graduate this academic year.

Interactions

Seminars by Prof. Kevrekidis: Several seminars at Universities (~30) and National Labs (~4), several invited/plenary talks (~30) and presentations at conferences (~50); Visits and discussions with UTRC personnel involved interactions with Drs. Dorobantu and Jacobson (complex system modeling techniques, model reduction in computational chemistry, also work on fuel cell dynamics modeling).

Transitions

A computational materials science company (CFDRC in Alabama) has used algorithms developed through this work with success in modeling fabrication of different types of CNT.

Honors/Awards

Crawford Prize of SIAM/Dynamical Systems (2003); Plenary lecture, SIAM Dynamical Systems meeting (2003); Plenary lecture, SIAM annual meeting, (2004); Plenary lecture, joint SIAM/SMB meeting (2006); NAS meeting (2005); also internationally (Bristol University, UK, the Weizmann Institute, Israel); Guggenheim Fellowship (precisely for the work on equation-free modeling of multiscale/complex systems performed under this grant, 2005). Moore Distinguished Fellowship at Caltech (2005). There was a full page article in SIAM News about this research program in 2005; also the PI was asked to join the Advisory Board of the Center for Cell Dynamics (at the Friday Harbor Lab, Univ. of Washington).

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